Splitting methods for the time dependent Schrödinger equation

S. Blanes,

Joint work with F. Casas and A. Murua

Instituto de Matemática Multidisciplinar
Universidad Politécnica de Valencia, SPAIN

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The Schrödinger equation

Consider the autonomous time dependent SE

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\nabla^2 + V(x)\right)\psi(x,t)$$

It is separable in its kinetic and potential parts. The solution of the discretised equation is given by

$$i\,\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t) \quad \Rightarrow \quad \mathbf{c}(t) = e^{-it\mathbf{H}}\mathbf{c}(0)$$

where $\mathbf{c} = (c_1,\ldots, c_N)^T \in \mathbb{C}^N$ and $\mathbf{H} = \mathbf{T} + \mathbf{V} \in \mathbb{R}^{N\times N}$ Hermitian matrix. Fourier methods are frequently used

$$(\mathbf{V}\mathbf{c})_i = V(x_i)c_i \qquad N \text{ products}$$
$$\mathbf{T}\mathbf{c} = \mathcal{F}^{-1}\mathbf{D}_T\,\mathcal{F}\mathbf{c} \qquad \mathcal{O}(N\log N) \text{ operations}$$

$\mathcal{F}$ is the fast Fourier transform (FFT)

Consider the Strang-splitting or leap-frog second order method

$$U_2(\tau) \equiv e^{\tau/2\mathbf{V}}\, e^{\tau\mathbf{T}}\, e^{\tau/2\mathbf{V}}$$

Notice that

$$\left(e^{\tau\mathbf{V}}\mathbf{c}\right)_i = e^{\tau V(x_i)} c_i$$

the exponentials are computed only once and are stored at the beginning. Similarly, for the kinetic part we have

$$e^{\tau\mathbf{T}}\mathbf{c} = \mathcal{F}^{-1} e^{\tau\mathbf{D}_T} \mathcal{F}\mathbf{c}$$

This splitting was proposed in:

Feit, Fleck, and Steiger, J. Comput. Phys., 47 (1982), 412.

$$\mathbf{U}_n(h) = \mathbf{U}_2(\beta_k h) \cdots \mathbf{U}_2(\beta_2 h)\, \mathbf{U}_2(\beta_1 h)$$

$$\begin{aligned} \mathbf{U}_n(h) &= e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}} \\ &= \Phi_1^*(d_k h)\Phi_1(c_k h) \;\cdots\; \Phi_1^*(d_1 h)\Phi_1(c_1 h) \end{aligned}$$

$$\mathbf{U}_n(h) = e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}} \qquad [\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0$$

$$\mathbf{U}_n(h) = e^{\tilde{\mathrm{B}}(h,\mathrm{b})}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{\tilde{\mathrm{B}}(h,\mathrm{b})}\, e^{ha_1 \mathrm{A}} \qquad [\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0$$

$$\mathbf{U}_n(h) = e^{hb_k \mathbf{H}_0}\, e^{\epsilon h a_k \mathbf{H}_1} \;\ldots\; e^{hb_1 \mathbf{H}_0}\, e^{\epsilon h a_1 \mathbf{H}_1} \qquad \|\epsilon \mathbf{H}_1\| \ll \|\mathbf{H}_0\|$$

$$\mathbf{U}_n(h) = e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}} \qquad \begin{aligned} &[\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0 \\ &[\mathrm{A},[\mathrm{A},[\mathrm{A},\mathrm{B}]]] = 0 \end{aligned}$$

$$\mathbf{U}_n = \mathbf{U}_P \mathbf{U}_K \mathbf{U}_P^{-1} \quad \Longrightarrow \quad \mathbf{U}_n^p = \mathbf{U}_P \mathbf{U}_K^p \mathbf{U}_P^{-1}$$

Non-autonomous Separable System

Let us now consider the non-autonomous separable system

$$\dot{\mathbf{u}} = (\mathbf{A}(\mathbf{t}) + \mathbf{B}(\mathbf{t}))\,\mathbf{u}$$

with the standard form to convert the system into autonomous

$$\frac{d}{dt}\underbrace{\begin{Bmatrix}\mathbf{u}\\ t_A\\ t_B\end{Bmatrix}}_{\mathbf{y}} = \underbrace{\begin{Bmatrix}\mathbf{A}(t_B)\mathbf{u}\\ 1\\ 0\end{Bmatrix}}_{\bar{\mathbf{A}}\mathbf{y}} + \underbrace{\begin{Bmatrix}\mathbf{B}(t_A)\mathbf{u}\\ 0\\ 1\end{Bmatrix}}_{\bar{\mathbf{B}}\mathbf{y}}$$

or, equivalently

$$\dot{\mathbf{y}} = \left(\bar{\mathbf{A}} + \bar{\mathbf{B}}\right)\mathbf{y}$$

This simple procedure can cause serious drawbacks in the numerical schemes to be used

Splitting Methods

$$\mathbf{U}_n(h) = \mathbf{U}_2(\beta_k h) \cdots \mathbf{U}_2(\beta_2 h)\, \mathbf{U}_2(\beta_1 h)$$

$$\begin{aligned} \mathbf{U}_n(h) &= e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}} \\ &= \Phi_1^*(d_k h)\Phi_1(c_k h) \;\cdots\; \Phi_1^*(d_1 h)\Phi_1(c_1 h) \end{aligned}$$

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$$\mathbf{U}_n(h) = e^{\tilde{\mathrm{B}}(h,\mathrm{b})}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{\tilde{\mathrm{B}}(h,\mathrm{b})}\, e^{ha_1 \mathrm{A}} \qquad [\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0$$

$$\mathbf{U}_n(h) = e^{hb_k \mathbf{H}_0}\, e^{\epsilon h a_k \mathbf{H}_1} \;\ldots\; e^{hb_1 \mathbf{H}_0}\, e^{\epsilon h a_1 \mathbf{H}_1} \qquad \|\epsilon \mathbf{H}_1\| \ll \|\mathbf{H}_0\|$$

$$\mathbf{U}_n(h) = e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}} \qquad \begin{aligned} &[\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0 \\ &[\mathrm{A},[\mathrm{A},[\mathrm{A},\mathrm{B}]]] = 0 \end{aligned}$$

$$\mathbf{U}_n = \mathbf{U}_P \mathbf{U}_K \mathbf{U}_P^{-1} \quad \Longrightarrow \quad \mathbf{U}_n^p = \mathbf{U}_P \mathbf{U}_K^p \mathbf{U}_P^{-1}$$

Splitting Methods

$$\mathbf{U}_n(h) = \mathbf{U}_2(\beta_k h) \cdots \mathbf{U}_2(\beta_2 h)\, \mathbf{U}_2(\beta_1 h)$$

$$\begin{aligned} \mathbf{U}_n(h) &= e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}} \\ &= \Phi_1^*(d_k h)\Phi_1(c_k h) \;\cdots\; \Phi_1^*(d_1 h)\Phi_1(c_1 h) \end{aligned}$$

$$\mathbf{U}_n(h) = e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}}$$

~~$[\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0$~~

$$\mathbf{U}_n(h) = e^{\tilde{\mathrm{B}}(h,\mathrm{b})}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{\tilde{\mathrm{B}}(h,\mathrm{b})}\, e^{ha_1 \mathrm{A}}$$

~~$[\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0$~~

$$\mathbf{U}_n(h) = e^{hb_k \mathbf{H}_0}\, e^{\epsilon h a_k \mathbf{H}_1} \;\ldots\; e^{hb_1 \mathbf{H}_0}\, e^{\epsilon h a_1 \mathbf{H}_1}$$

~~$\|\epsilon \mathbf{H}_1\| \ll \|\mathbf{H}_0\|$~~

$$\mathbf{U}_n(h) = e^{hb_k \mathrm{B}}\, e^{ha_k \mathrm{A}} \;\ldots\; e^{hb_1 \mathrm{B}}\, e^{ha_1 \mathrm{A}}$$

~~$[\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0$~~
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$$\mathbf{U}_n = \mathbf{U}_P \mathbf{U}_K \mathbf{U}_P^{-1} \quad \Longrightarrow \quad \mathbf{U}_n^p = \mathbf{U}_P \mathbf{U}_K^p \mathbf{U}_P^{-1}$$

Problem: $H(q,p,t) = \frac{1}{2}p^2 + \frac{1}{2}f(t)q^2 + \varepsilon \sum_{j=1}^{s} \cos(q - \omega_j t)$

describes the motion of a charged particle in a magnetic field perturbed by s electrostatic plane waves, each with the same wavenumber and amplitude, but with different temporal frequencies.

Standard split

$$H = \left(\frac{1}{2}p^2 + \frac{1}{2}f(t_B)q^2 + \lambda_A\right) + \left(\varepsilon \sum_{j=1}^{s} \cos(q - \omega_j t_A) - \lambda_B\right)$$

Our split

$$H = \left(\frac{1}{2}p^2 + \frac{1}{2}f(t_A)q^2 + \lambda_A\right) + \varepsilon \sum_{j=1}^{s} \cos(q - \omega_j t_A)$$

This split allows to use methods for near-integrable systems in addition
To techniques for RKN methods included modified potentials and Processing

SB, F. Diele, C. Marangi, and S. Ragni, **Splitting and composition methods for explicit time dependence in separable dynamical systems**.
JCAM 235 (**2010**) 646-659.

Polynomial Approximations: Taylor, Chebyshev and Splitting

Let us consider again the linear time dependent SE

$$i\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t) \quad \Rightarrow \quad \mathbf{c}(t) = e^{-it\mathbf{H}}\mathbf{c}(0)$$

with $\mathbf{H}$ real and symmetric.
This problem can be reformulated using real variables.

Consider $\mathbf{c} = \mathbf{q} + i\mathbf{p}$ then $i\frac{d}{dt}(\mathbf{q} + i\mathbf{p}) = \mathbf{H}(\mathbf{q} + i\mathbf{p})$

Hamiltonian system: $\mathcal{H} = \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} + \frac{1}{2}\mathbf{q}^T\mathbf{H}\mathbf{q}$

$$\frac{d}{dt}\begin{Bmatrix}\mathbf{q}\\ \mathbf{p}\end{Bmatrix} = \begin{pmatrix}0 & \mathbf{H}\\ -\mathbf{H} & 0\end{pmatrix}\begin{Bmatrix}\mathbf{q}\\ \mathbf{p}\end{Bmatrix}$$

or, in short: $z' = M\,z$ with $z = (\mathbf{q},\mathbf{p})^{\mathrm{T}}$

Formal solution: $$\mathbf{O}(t) = \begin{pmatrix}\cos(t\mathbf{H}) & \sin(t\mathbf{H})\\ -\sin(t\mathbf{H}) & \cos(t\mathbf{H})\end{pmatrix}$$

The Taylor Method

An m-stage Taylor method for solving the linear equation can be written as

$$z_{n+1} = P_m^T(\tau M) z_n$$

where $P_m^T(\tau M)$ is the Taylor expansion of the exponential. It is a polynomial function of degree m which approximates the exact solution up to order m

$$P_m^T(\tau M) \equiv \sum_{j=0}^{m} \frac{1}{j!}(\tau M)^j = e^{\tau M} + \mathcal{O}(\tau^{m+1})$$

and we can advance each step by using the Horner's algorithm

$$\begin{aligned}
&y_0 = z_n \\
&\textbf{do} \quad i = 1, m \\
&\quad y_i = \tfrac{1}{i} \tau M y_{i-1} \\
&\quad z_n = z_n + y_i \\
&\textbf{enddo} \\
&z_{n+1} = y_m
\end{aligned}$$

This algorithm can be trivially rewritten in terms of the real vectors, $\mathbf{q}$,$\mathbf{p}$, and it only requires to store two extra vector $\mathbf{q}$ and $\mathbf{p}$.

The Taylor Method

The matrix $P_m^T(\tau M)$ that propagates the numerical solution can be written as

$$P_m^T(\tau H) = \begin{pmatrix} T_1(\tau H) & T_2(\tau H) \\ -T_2(\tau H) & T_1(\tau H) \end{pmatrix}$$

where the entries $T_1(y)$ and $T_2(y)$ are the Taylor series expansion of cos(y) and sin(y) up to order m, i.e.

$$P_1^T(x) = \begin{pmatrix} 1 & x \\ -x & 1 \end{pmatrix}, \qquad P_2^T(x) = \begin{pmatrix} 1 - \frac{x^2}{2} & x \\ -x & 1 - \frac{x^2}{2} \end{pmatrix}$$

Notice that $\det P_m^T(y) = T_1(y)^2 + T_2(y)^2 \neq 1$
it is not a symplectic transformation! The eigenvalues are given by

$$\lambda_{\pm}^T = T_1 \pm iT_2$$

The scheme is stable if $T_1^2(y) + T_2^2(y) \leq 1$

For practical purposes, we require however

$$T_1^2(y) + T_2^2(y) \leq 1 + tol$$

The Chebyshev Method

The Chebyshev method approximates the action of the exponential on the initial conditions by a near-optimal polynomial given by:

$$u(t) = \mathrm{e}^{-itH}\, u_0 \approx P_m^C(tH)\, u_0$$

where

$$P_{m-1}^C(tH)u_0 = c_0 u_0 + 2\sum_{k=1}^{m} c_k T_k\left(\frac{H}{\rho(H)}\right) u_0$$

with $c_k = (-i)^k J_k(t\,\rho(H))$. Here, $T_k(x)$ is the kth Chebyshev polynomial generated from the recursion

$$T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x), \qquad k \geq 1$$

and $T_0(x)$=1, $T_1(x)$=x. $J_k(w)$ are the Bessel functions of the first kind which provides a superlinear convergence for $m > w$ or, in other words, when

$$\frac{t\rho(H)}{m} \leq 1$$

The Chebyshev Method

The Clenshaw algorithm allows to compute the action of the polynomial by storing only two vectors

$$
\begin{aligned}
& d_{m+1} = 0, \qquad d_m = 0 \\
& \textbf{do} \quad i = m-1, 0 \\
& \quad d_i = c_i z_n + \frac{2}{\rho(H)} H d_{i+1} - d_{i+2} \\
& \textbf{enddo} \\
& z_{n+1} = d_0 - d_2
\end{aligned}
$$

which can also be easily rewritten in term of the real vectors **q,p**.

The scheme can be written as

$$
P_m^C(\tau H) = \begin{pmatrix} C_1(\tau H) & C_2(\tau H) \\ -C_2(\tau H) & C_1(\tau H) \end{pmatrix}
$$

As in the Taylor case: $\det P_m^C(y) = C_1(y)^2 + C_2(y)^2 \neq 1$

It is not a symplectic transformation.

The Symplectic Splitting Method

We have built splitting methods for the harmonic oscillator!!!

$$\frac{d}{dt}\begin{Bmatrix} q \\ p \end{Bmatrix} = \Big[\underbrace{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}_{A} + \underbrace{\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}}_{B}\Big]\begin{Bmatrix} q \\ p \end{Bmatrix}$$

Exact solution (ortogonal and symplectic)

$$O(t) = \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix}$$

We consider the composition

$$K(h) \equiv \prod_{i=1}^{m} e^{ha_i A}\, e^{hb_i B}$$

Notice that

$$e^{hA}\, e^{hB} = \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -h & 1 \end{pmatrix} = \begin{pmatrix} 1-h^2 & h \\ -h & 1 \end{pmatrix}$$

The Symplectic Splitting Method

We have $$K(h) \equiv \prod_{i=1}^{m} \begin{pmatrix} 1 - a_i b_i h^2 & a_i h \\ -b_i h & 1 \end{pmatrix} = \begin{pmatrix} K_1 & K_2 \\ K_3 & K_4 \end{pmatrix}$$

$$K_1 = \sum_{i=0}^{m} k_{1,i} h^{2i} \qquad K_2 = \sum_{i=1}^{m} k_{2,i} h^{2i-1}$$
$$K_3 = \sum_{i=1}^{m} k_{3,i} h^{2i-1} \qquad K_4 = \sum_{i=0}^{m} k_{4,i} h^{2i}$$

which are polynomials of degree twice higher as in the previous cases for the same number of stages.

The algorithm: a **generalisation** of the Horner's algorithm or the Clenshav algorithm

$$\begin{aligned} \mathbf{do} \quad & i = 1, m \\ & v = Hp \\ & q := q + a_i \tau v \\ & v = Hq \\ & p := p - b_i \tau v \\ \mathbf{enddo} & \end{aligned}$$

It only requires to store one additional real vector of dimension

The Symplectic Splitting Method

The methods preserve symplecticity by construction: $\det K(h) = 1$

Stability: M is stable if $|\mathrm{Tr}\ K|<2$, i.e.

$$|K_1 + K_4| = \left| \sum_{i=0}^{m} \left(k_{1,i} + k_{4,i}\right) h^{2i} \right| < 2$$

Theorem:Any composition method is conjugate to an orthogonal method, and unitarity is preserved up to conjugacy.

There is a recursive procedure to get the coefficients of the splitting methods from the coefficients of the matrix K.

We can build different matrices with:
- Large stability domain
- Accurate approximation to the solution in the whole interval (like Chebyshev)
- Methods with different orders of accuracy and very large number of satges.

Taylor	order	tol=inf	tol=10-8	tol=10-4
	10.	0.	0.	0.
	15.	0.111249	0.111249	0.111249
	20.	0.164515	0.164515	0.164515
	25.	0.	0.065246	0.065246
	30.	0.	0.108088	0.108088
	35.	0.0461259	0.138361	0.322661
	40.	0.0804521	0.160884	0.321618
	45.	0.	0.178294	0.320804
	50.	0.	0.192154	0.32015

Chebyshev	order	tol=inf	tol=10-8	tol=10-4
	20.	0.00362818	0.321723	0.643217
	25.	0.00233368	0.384289	0.64029
	30.	0.00162599	0.425648	0.638324
	35.	0.00119743	0.45502	0.636912
	40.	0.000918402	0.476957	0.63585
	45.	0.000726646	0.635021	0.635021
	50.	0.000589228	0.634356	0.634356
	55.	0.	0.633812	0.633812
	60.	0.	0.633357	0.633357

Splitting methods

m	r	θ'	y_*/m	$\sum_j(\lvert a_j\rvert+\lvert b_j\rvert)$	$\mu_r(\theta' m)$	$\nu_r(\theta' m)$
20	16	1	1.0456	3.0553	0.000611028	0.0258433
30	24	1	1.0246	3.19658	0.0000841871	0.0373544
30	0	1	1.1411	3.04948	$2.91902 \cdot 10^{-13}$	$2.28673 \cdot 10^{-9}$
30	0	0.75	1.027	3.44381	$1.2545 \cdot 10^{-17}$	$5.96706 \cdot 10^{-14}$
40	0	1	1.15953	3.21986	$1.06301 \cdot 10^{-15}$	$1.07587 \cdot 10^{-12}$
30	6	1.4	1.41876	3.0921	0.0000518519	0.0131295

Error bounds

$$\|u_n - u(t)\| \leq \frac{|t|\,\mu_k(\theta)\,\|u_0\|_{k+1} + \nu_k(\theta)\|u_0\|_k}{\rho(H)^k}.$$

Schrödinger equation with a Poschl-Teller potential

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t)$$

with

$$V(x) = -\frac{\alpha^2}{2\mu}\frac{\lambda(\lambda-1)}{\cosh^2(\alpha x)}$$

$$\mu = 1745, \quad \alpha = 2, \quad \lambda = 24{,}5,$$

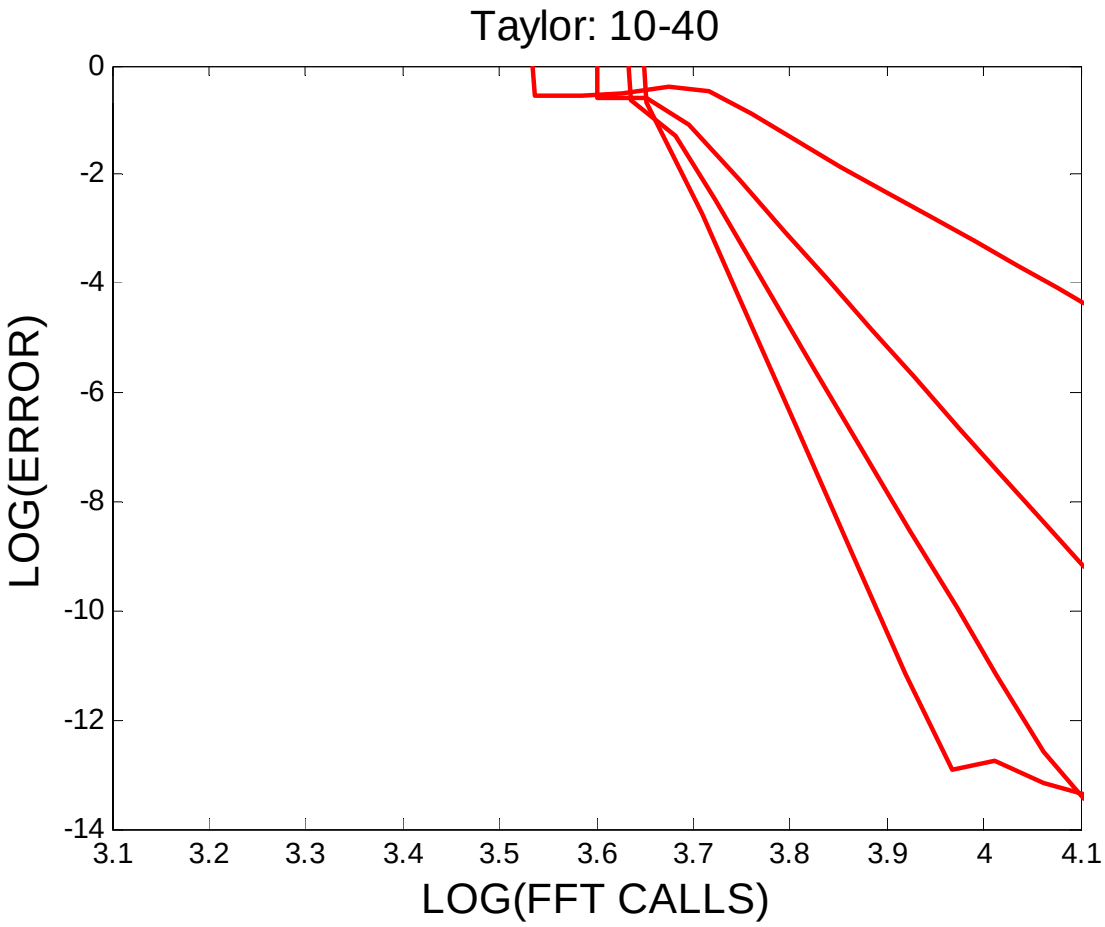
Initial conditions

$$\psi(x,0) = \rho e^{-9^2 x^2}$$

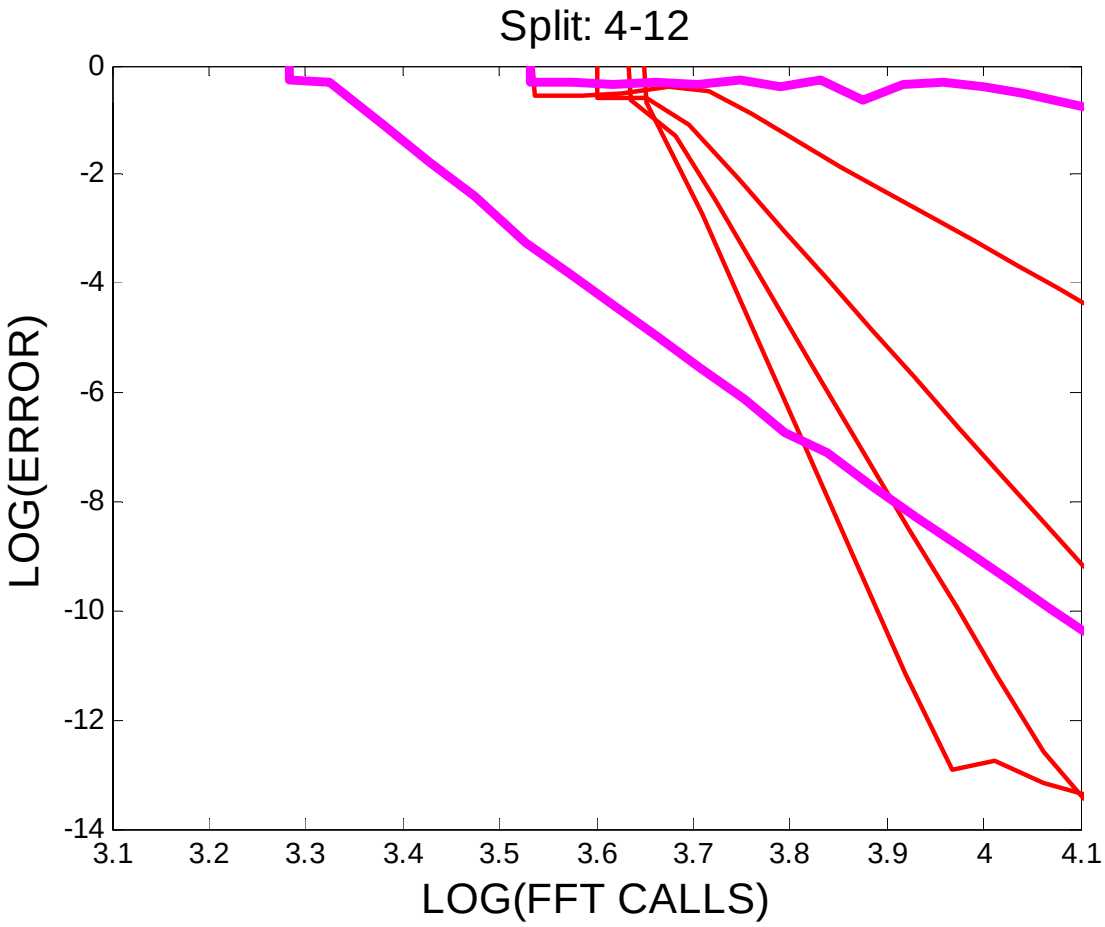
$$t \in [0, 2T] \;\; x \in [-5,5], \quad N = 128 \text{ parts}$$

$$\rho(H) \simeq \frac{1}{2\mu}\left(\frac{\pi}{\Delta x}\right)^2 + (V_{max} - V_{min}) = 1.12$$

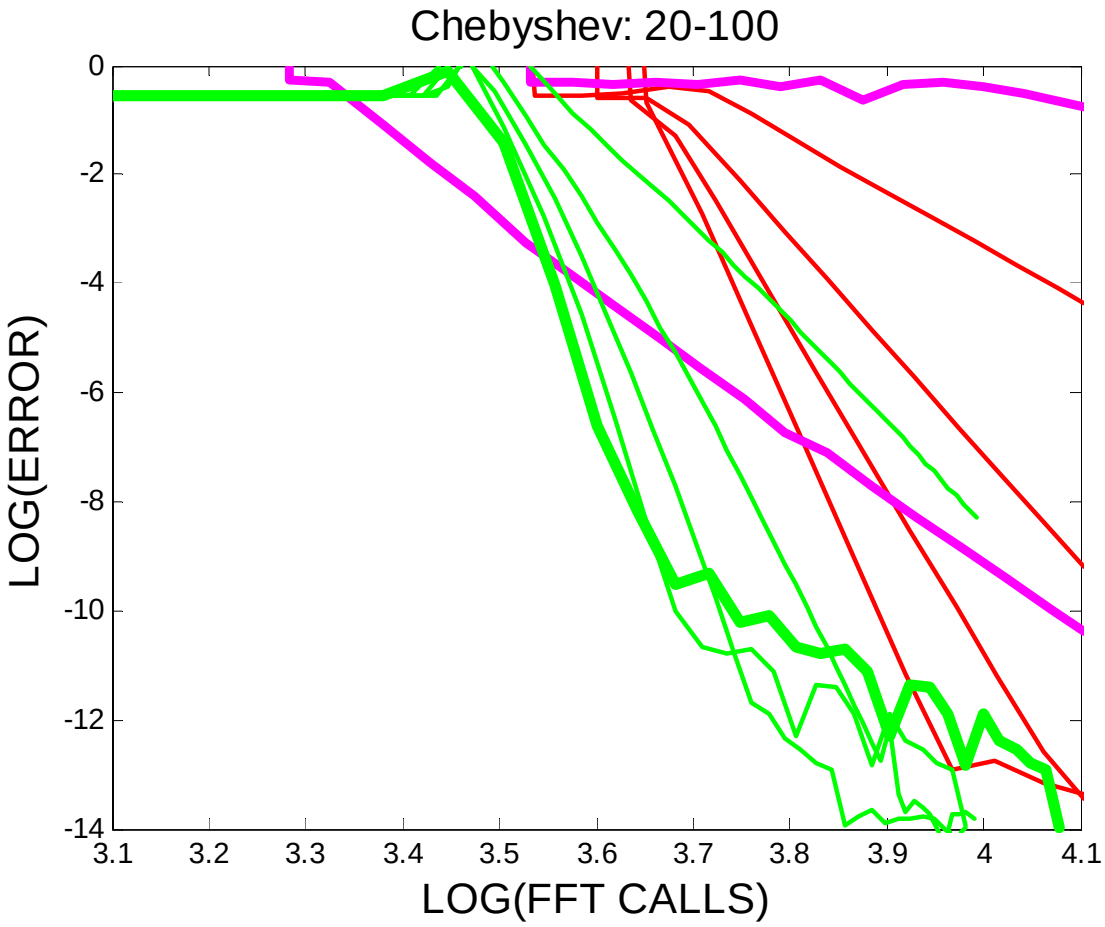
Poschl-Teller potential



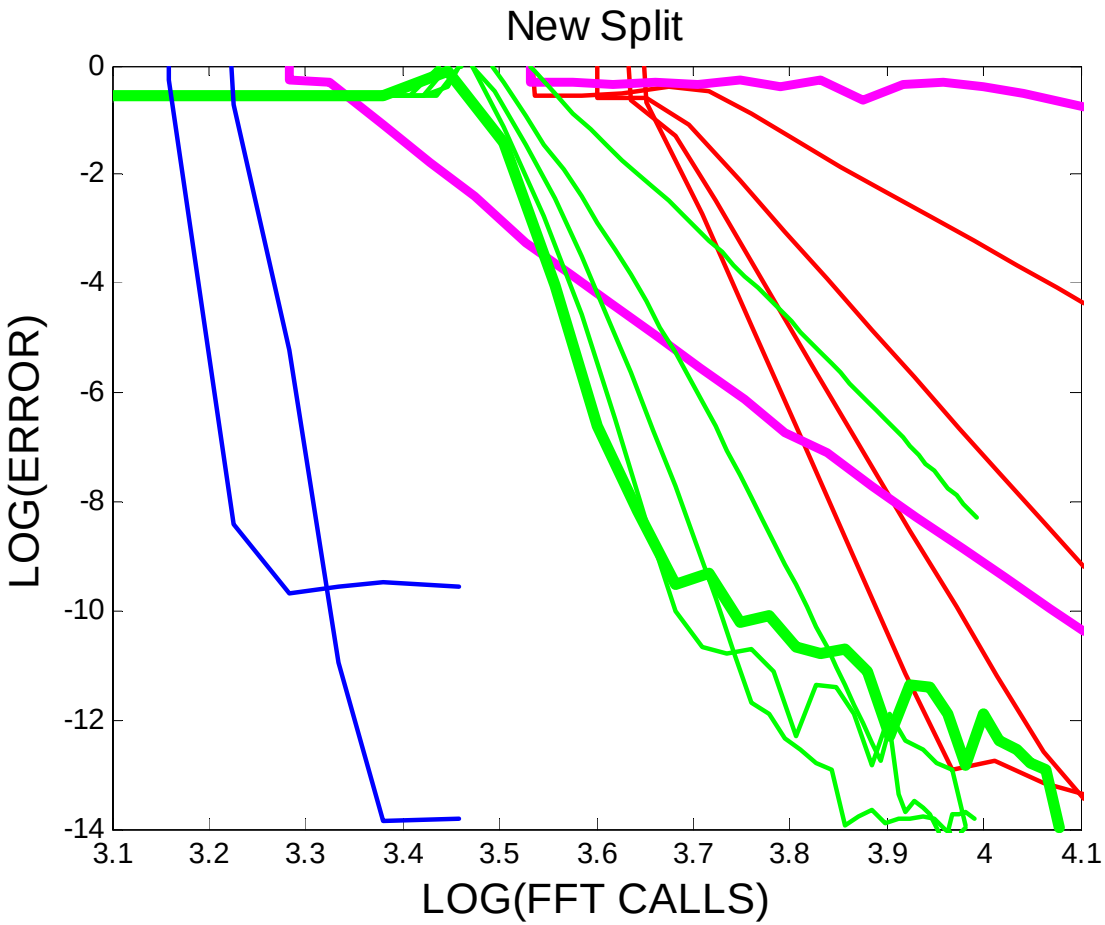
Poschl-Teller potential



Poschl-Teller potential



Poschl-Teller potential



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Group webpage: http://www.gicas.uji.es

SB, F. Casas and A. Murua, **On the linear stabylity of splitting methods**, Found. Comp. Math., 8 (2008), 357-393.

SB, F. Casas and A. Murua, **Symplectic splitting operator methods for the time-dependent Schrödinger equation**, J. Chem. Phys. 124 (2006) 234105.

Problem: To numerically solve the linear time dependent system

$$x' = M(t)y, \qquad y' = -N(t)x$$

It can appear after discretisation of linear PDEs (or their linear part): linear and non-linear Schrödinger equation, Maxwell equations, etc.

The simplest solution is to convert the system into autonomous

$$\begin{aligned} x' &= M(y_t)y & y' &= -N(x_t)x \\ x'_t &= 1 & y'_t &= 1 \end{aligned}$$

where $x_t, y_t \in \mathbb{R}$ The system is no longer linear and the most efficient methods can not be used

$$[\mathrm{B},[\mathrm{B},[\mathrm{B},\mathrm{A}]]] = 0$$
$$[\mathrm{A},[\mathrm{A},[\mathrm{A},\mathrm{B}]]] = 0$$

The Magnus series expansion

Theorem (Magnus 1954). Let $A(t)$ be a known function of t (in general, in an associative ring), and let $Y(t)$ be an unknown function satisfying $Y' = A(t)\ Y$, with $Y(0) = I$. Then, if certain unspecified conditions of convergence are satisfied, $Y(t)$ can be written in the form

$$Y(t) = \exp \Omega(t),$$

where

$$\frac{d\Omega}{dt} = \sum_{n=0}^{\infty} \frac{B_n}{n!} \operatorname{ad}_{\Omega}^{n} A,$$

and B_n are the Bernouilli numbers.

The convergence is asured if $\|\Omega\| < \pi$

The Magnus expansion

$$X(t) = e^{\Omega(t)} X_0, \qquad \Omega = \sum_{k=1}^{\infty} \Omega_k$$

which can be obtained by Picard iteration or using a recursive formula

$$\begin{aligned}
\Omega_1 &= \int_0^t A(t)dt \\
\Omega_2 &= \frac{1}{2}\int_0^t dt_1 \int_0^{t_1} dt_2 [A_1, A_2] \\
\Omega_3 &= \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \{\ [A_1, A_2, A_3] + [A_3, A_2, A_1]\ \} \\
\Omega_4 &= \frac{1}{12}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \{\ [A_1, A_4, A_3, A_2] \\
&\quad + [A_2, A_3, A_4, A_1] + [A_1, A_2, A_3, A_4] - [A_4, A_3, A_2, A_1]\ \}
\end{aligned}$$

where $A_i \equiv A(t_i)$, $[A_1, A_2, A_3] \equiv [A_1, [A_2, A_3]]$

Convergence condition: $\int_0^t \|A(s)\|_2 ds < \pi$

This is a sufficient but NOT necessary condition

F. Casas, Sufficient conditions for the convergence of the Magnus expansion, J. Phys. A, 40 (2007), 15001-15017

Splitting-Magnus methods

$$z' = \Big(A(t) + B(t)\Big) z$$

with

$$A(t) = \begin{pmatrix} 0 & H(t) \\ 0 & 0 \end{pmatrix}, \quad B(t) = \begin{pmatrix} 0 & 0 \\ -H(t) & 0 \end{pmatrix}$$

Splitting-Magnus methods

$$z' = \Big(A(t) + B(t)\Big) z$$

with

$$A(t) = \begin{pmatrix} 0 & H(t) \\ 0 & 0 \end{pmatrix}, \quad B(t) = \begin{pmatrix} 0 & 0 \\ -H(t) & 0 \end{pmatrix}$$

We can approximate the solution by the composition

$$K(t,h) = e^{A_m(t,h)} e^{B_m(t,h)} \cdots e^{A_1(t,h)} e^{B_1(t,h)}$$

$$= \begin{pmatrix} I & M_m \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_m & I \end{pmatrix} \cdots \begin{pmatrix} I & M_1 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_1 & I \end{pmatrix}$$

Splitting-Magnus methods

$$z' = \Big(A(t) + B(t)\Big) z$$

with

$$A(t) = \begin{pmatrix} 0 & H(t) \\ 0 & 0 \end{pmatrix}, \quad B(t) = \begin{pmatrix} 0 & 0 \\ -H(t) & 0 \end{pmatrix}$$

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with the averages

$$M_i = h \sum_{j=1}^{k} \rho_{ij} H(t + c_j h), \quad N_i = h \sum_{j=1}^{k} \sigma_{ij} H(t + c_j h)$$

SB, F. Casas and A. Murua, Splitting methods for non-autonomous Linear systems, Int. Jour. Comp. Math., 6 (2007), 713-727

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This technique can be useful for methods up to order six and for moderate accuracies.

For more accurate results and higher order methods one can use a symmetric second order scheme and the multiproduct methods

Siu A. Chin: http://faculty.physics.tamu.edu/chin

Conclusions

- Splitting methods are powerful tools for numerically solving the Schrödinger equation
- The performance strongly dependes on how the system has been split as well as on the choice of the appropriate methods for each problem
- Alternatively, one can build methods tailored for particular problems
- There are many interesting open problems